Quantum stochastic description of collisions in a canonical Bose gas

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We derive a stochastic process that describes the kinetics of a one-dimensional Bose gas in a regime where three body collisions are important. In this situation the system becomes non integrable offering the possibility to investigate dissipative phenomena more simply compared to higher dimensional gases. Unlike the quantum Boltzmann equation describing the average momentum distribution, the stochastic approach allows a description of higher-order correlation functions in a canonical ensemble. As will be shown, this ensemble differs drastically from the grand canonical one. We illustrate the use of this method by determining the time evolution of the momentum mode particle number distribution and the static structure factor during the evaporative cooling process.

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The stochastic kinetic description of a quantum gas has been the subject of considerable activity [1–3]. The main idea is to describe the state in terms of a set of stochastic classical fields $\psi^{(i)}(r,t)$ $(i=1,...,I)$ associated to the bosonic quantum field $\psi(r,t)$ whose averages give access to the n-point correlation functions, possibly in the CN (canonical) ensemble. The determination of these quantities has been shown to be of relevance in recent interference experiments with cold atoms[4] where mode probability functions have triggered considerable interest [5, 6]. As discussed in [1], the main difficulty is to be able to derive an associated Fokker-Planck(FP)-like equation for the probability in the P representation which can be recasted into a stochastic Langevin equation. Such a task cannot be achieved exactly since the resulting equation would be a non dissipative FP equation [1, 7–9]. Only the use of the positive P representation appears to be tractable [9]. Some approximations have to be made in a bid to obtain numerically solvable dissipative equations. For the general case of finite temperature, only a phenomenological approach is available in which the stochastic terms guarantee the approach towards thermodynamic equilibrium without the requirement of an additional cutoff at large momentum [3].

In this Letter, we present a microscopic derivation of a Langevin equation starting from the full many body Hamiltonian in which the stochasticity originates from collision processes. For simplicity, we study a one dimensional Bose gas subject to three-body interactions only (two-body interactions does not lead to effective thermalization in 1D). Such a system could be realized in cold atom experiments [10] and differs from the usual 1D exactly solvable Hamiltonian by the addition to the two-body quartic term of a sixtic interaction term resulting from virtual interaction with transverse degrees of freedom. Its study allows simpler access to the exploration of quantum collisions compared to the more involved higher dimensional systems [2, 11, 12], in particular to the study of their enhancement due to the Bose statistics. As an illustration, we consider the dynamics of evaporative cooling in the CN ensemble and show that the time evolution of quantities such as correlations or mode probability distribution differ strongly from the one obtained from the Boltzmann equation valid only in the grand canonical (GN) ensemble.

Defining the atom mass m, the scattering length α_s, its 1D density n and the transverse trap frequency ω_r, we focus on the thermalization regime described in [10] characterized by a high transverse confinement $\hbar\omega_r \gg k_B T$, a weak correlation parameter $\gamma = 2\alpha_s m\omega_r/\hbar n \ll 1$ in order to violate integrability so that the three-body collision rate overcomes the two-body collision rate responsible for transverse mode excitations.

Restricting ourselves to a uniform gas and defining the spatial Fourier components of the field $\psi^{(i)}(r,t) = \sum_k \exp(ikr)\alpha_k^{(i)}(t)/\sqrt{L}$, we shall show how to derive the following Langevin-type equation:

$$d\alpha_p^{(i)} = (\Gamma_p^{in} - \Gamma_p^{out} + i\omega_p')\alpha_p^{(i)}dt + \sqrt{2\Gamma_p^{in}}d\eta_p^{(i)} \quad (1)$$

where ω_p' is the kinetic and mean field energy of the atom, $\Gamma_p^{in}(t)$ and $\Gamma_p^{out}(t)$ correspond to the ingoing and outgoing collision terms respectively. These are averaged functionals of the $\alpha_p^{(i)}(t)$ and are determined from Eq.(17,18). The noise $d\eta_p^{(i)}$ follows a Gaussian distribution with the only non trivial average $\langle d\eta_p d\eta_{p'}^*\rangle = \delta_{p,p'}dt$. In contrast to [2, 7], this equation includes both high and low energy modes in the stochastic process. The average is defined as $\langle A\rangle = \sum_{i=1}^I A^{(i)}/I$ for any set of realization $A^{(i)}$. It is done in the grand canonical (GC) ensemble and corresponds to the Monte-Carlo approximation of the integral over coherent state labeled by the α_p's [3]. In other words, the expectation value of any observable functional of the creation annihilation operator $a_p^\dagger$ and a_p, is in the limit of a large set I, identical to an average over the stochastic variables α_p^* and α_p.

We note the connection with the quantum Boltzmann equation. Multiplying (1) by its complex conjugate and taking the average over the ensemble, the stochastic equation is connected to the quantum Boltzmann equa-

tion for the momentum distribution $\overline{n}_k = \langle n_k \rangle = \langle |\alpha_k|^2 \rangle$:

$$\frac{d\overline{n}_k(t)}{dt} = 2\Gamma_k^{in}(1+\overline{n}_k) - 2\Gamma_k^{out}\overline{n}_k \tag{2}$$

This equation becomes closed if the Γ_k^{in} and Γ_k^{out} are functionals of $\overline{n}_k$. This is realized through the application of the Wick's decomposition theorem (which corresponds to the stosszahlansatz): defining the product $M_n(\{\alpha_k\}) = \alpha^*_{k_1} \dots \alpha^*_{k_n} \alpha_{k'_1} \dots \alpha_{k'_n}$, its average in the GC ensemble for a uniform gas is decomposed as:

$$\langle M_n(\{\alpha_k\}) \rangle = \overline{n}_{k_1} \dots \overline{n}_{k_n} \sum_{\{k_j\} \in P} \prod_i \delta_{k_i,k_j} \tag{3}$$

where P is the permutation ensemble. On the contrary, the stosszahlansatz is not necessary anymore in Eq.(1) and correlations can be taken into account.

Another advantage of the stochastic formalism is the possibility to relate the averages in the CN ensemble to the GC ones by means of the weight functions $W_N(\{\alpha_k\}) = e^{-\sum_k |\alpha_k|^2} \left(\sum_k |\alpha_k|^2\right)^N / N!$ so that for N atoms we obtain for any product [3]:

$$\langle M_n(\{\alpha_k\}) \rangle_N = \frac{\langle W_{N-n}(\{\alpha_k\}) M_n(\{\alpha_k\}) \rangle}{\langle W_N(\{\alpha_k\}) \rangle} \tag{4}$$

The weight function plays the role of a projection operator restricting the particle number to N. Probability distribution in the CN ensemble can also be determined for mode population. For example, defining the weight functions $W_{N,k\neq 0} = e^{-\sum_{k\neq 0} |\alpha_k|^2} \left(\sum_{k\neq 0} |\alpha_k|^2\right)^N / N!$ and $W_{N,k=0} = e^{-|\alpha_0|^2} |\alpha_0|^{2N} / N!$, the probability distribution for the zero momentum mode reads:

$$P_N(n_0) = \frac{\langle W_{N-n_0,k\neq 0}(\{\alpha_k\}) W_{n_0,k=0}(\{\alpha_k\}) \rangle}{\langle W_N(\{\alpha_k\}) \rangle} \tag{5}$$

The determination of the stochastic equation is done as follows. We start from the ternary many body Hamiltonian [10]:

$$H = \sum_k \omega_k c_k^\dagger c_k - \frac{g_3}{L^2} \sum_{\sum_i p_i = \sum_i q_i} c_{p_1}^\dagger c_{p_2}^\dagger c_{p_3}^\dagger c_{q_1} c_{q_2} c_{q_3} \tag{6}$$

where $\omega_k = k^2/2m$ is the atom kinetic energy and $g_3 = 2\ln(4/3)\hbar\omega_r \alpha_s^2$ is the ternary three body interactions. The suppression of the quartic interactions proportional to $g_2 = \hbar\omega_r \alpha_s$ is valid in a region where the mean field interaction energy is negligible compared to the kinetic energy i.e. $g_2 n \ll k_B T$ so that the phonon excitation energy are mostly particle-like [10]. Starting the density matrix $\rho(t)$, we obtain the reduced density matrix for the momentum mode p by taking the trace over all other modes:

$$\rho_p(t) = \mathrm{Tr}_{\setminus p}\left(\rho(t)\right) \tag{7}$$

The stochastic time evolution of the mode p is derived by considering the other modes as a bath for this mode. For

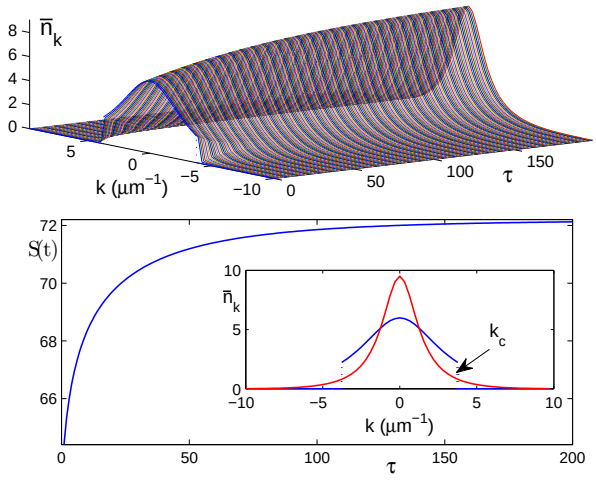

FIG. 1. Evolution of the momentum average distribution nk vs. the reduced time τ. The corresponding entropy is shown below and indicate how the distribution is close to equilibrium. Initial and final distributions are shown in blue and red respectively in the inset.

this purpose, we decompose the density matrix in terms of an uncorrelated contribution and a correlated one:

$$\rho(t) = \prod_p \rho_p(t) + \delta\rho(t) \tag{8}$$

The Hamiltonian can be decomposed into three terms:

$$H = H_1 + H_2 + H_3 \tag{9}$$

where $n_k = a_k^\dagger a_k$ and

$$H_1 = \omega_p n_p + \mathcal{O}(1/L) \tag{10}$$

$$H_2 = A_p n_p + C_p^\dagger a_p + a_p^\dagger C_p + \mathcal{O}(1/L) \tag{11}$$

and where A_p, C_p and H_3 are operators describing the other modes. We omit terms of the order $\mathcal{O}(1/L) \ll n$ which are negligible in the thermodynamic limit. Using the formalism in [8] to derive the master equation up to the second order in g_3, we obtain:

$$\begin{aligned}\frac{\partial \rho_p}{\partial t} = &-\frac{i}{\hbar}[H'_1, \rho_p] + \Gamma_p^{in}(t)(2a_p^\dagger \rho_p a_p - [a_p a_p^\dagger, \rho_p]_+) \\ &- \Gamma_p^{out}(t)([a_p^\dagger a_p, \rho_p]_+ - 2a_p \rho_p a_p^\dagger)\end{aligned} \tag{12}$$

where

$$H'_1 = H_1 + \mathrm{Tr}_{\setminus p}\left(\prod_{k\neq p} \rho_k H_2\right) = \omega'_p n_p \tag{13}$$

defining $\omega'_p = \omega_p - 3! g_3 n^2$ and $n = \sum_k \langle n_k \rangle / L$ and where

$$\begin{aligned}\Gamma_p^{in}(t) &= \mathrm{Re}\frac{1}{\hbar^2}\int_0^\infty dt' \langle C_p^\dagger(t') C_p \rangle \\ &= \mathrm{Re}\frac{1}{\hbar^2}\int_0^\infty dt' \mathrm{Tr}(C_p^\dagger(t') C_p \prod_{k\neq p} \rho_k(t))\end{aligned} \tag{14}$$

$$\Gamma_p^{out}(t) = \mathrm{Re}\frac{1}{\hbar^2}\int_0^\infty dt' \langle C_p(t') C_p^\dagger \rangle \tag{15}$$

Terms containing the operator A_p do not contribute up to g_3^2 by symmetry between the in and the out terms. The only contribution comes from the operator C_p which expressed in the interaction picture becomes:

$$C_{p_1}(t) = \frac{3g_3}{L^2} \sum_{\sum_i p_i = \sum_i q_i} e^{i\sum_i(\omega_{p_i}-\omega_{q_i})t} c^\dagger_{p_2} c^\dagger_{p_3} c_{q_1} c_{q_2} c_{q_3} \quad (16)$$

The stochastic equation can be implemented numerically directly using Eq.(14,15) but in order to avoid the summation over too many momentum variables we make the random phase approximation. For a uniform gas, we can neglect off-diagonal contributions in the p_i and q_i since they induce a phase factor that appears to be random and thus cancels in the summation process. Thus, only diagonal components remain. Carrying out the integral over t', we obtain with the following expression:

$$\Gamma^{in}_p(t) = (3!)^2\pi \left(\frac{g_3}{\hbar L^2}\right)^2 \sum_{\{p_i,q_i\}} \delta_{\sum_i p_i, \sum_i q_i} \delta(\sum_i \omega_{p_i} - \sum_i \omega_{q_i}) \langle n_{p_2} n_{p_3} (n_{q_1}+1)(n_{q_2}+1)(n_{q_3}+1)\rangle \quad (17)$$

$$\Gamma^{out}_p(t) = (3!)^2\pi \left(\frac{g_3}{\hbar L^2}\right)^2 \sum_{\{p_i,q_i\}} \delta_{\sum_i p_i, \sum_i q_i} \delta(\sum_i \omega_{p_i} - \sum_i \omega_{q_i}) \langle n_{q_1} n_{q_2} n_{q_3} (n_{p_2}+1)(n_{p_3}+1)\rangle \quad (18)$$

Note the Bose enhancement factor (terms $n_p + 1$) that amplifies the collision process when the output modes are already populated. From this form we can deduce the FP equation associated to the master equation (12):

$$\frac{\partial P_p(t)}{\partial t} = \left\{ -i\omega'_p \left(\alpha_p \frac{\partial}{\partial \alpha_p} - \alpha^*_p \frac{\partial}{\partial \alpha^*_p}\right) + (\Gamma^{out}_p(t) - \Gamma^{in}_p(t)) \left(\frac{\partial}{\partial \alpha_p}\alpha_p + \frac{\partial}{\partial \alpha^*_p}\alpha^*_p\right) + 2\Gamma^{in}_p(t) \frac{\partial}{\partial \alpha_p}\frac{\partial}{\partial \alpha^*_p} \right\} P_p(t) \quad (19)$$

from which we deduce the Langevin equation Eq.(1). The solution of this equation is a Gaussian distribution $P_p(t) = \exp(-|\alpha_p|^2/\overline{n}_p(t))/\overline{n}_p(t)$ with the normalization $\int d^2\alpha_p P_p(t)/\pi = 1$ and where $\overline{n}_p(t)$ has to fulfill Eq.(2). In equilibrium in the GC ensemble, through the application of Eq.(3) on Eq.(17,18), we recover the Bose-Einstein distribution $\overline{n}_k = 1/[\exp((\omega_p - \mu)/k_B T) - 1]$ as the stationary solution where the parameter μ defines the chemical potential.

For an illustration of all these considerations, we apply the stochastic method to the process of evaporative cooling. We take a gas of ^{87}Rb of $n = 5.25\,\mu m^{-1}$ confined in a box of size $L = 20\mu m$ with $\omega_r/2\pi = 6kHz$ and $\alpha_s = 5.3nm$. We choose the dimensionless time $\tau = 10^6 t/t^*$ where $1/t^* = (3!)^3 (g_3/\hbar L)^2 m/\pi\hbar$.

We start from an initial Bose gas at high temperature $T_i = 29nK$, we then remove the hottest atom with momentum higher than $k_c = 4\mu m^{-1}$ and study the relaxation process of this cut distribution towards an equilibrium one with a lower temperature $T_f = 9nK$ at a time estimated to $t = 0.14s$ ($\tau = 200$). The time evolution of the GC distribution calculated from Boltzmann approach of Eq.(2) is shown in Fig.1 together with the entropy $S(t) = \sum_p (\overline{n}_p+1)\log(\overline{n}_p+1) - \overline{n}_p \log(\overline{n}_p)$ evolution that allows to monitor the speed at which the equilibrium state is reached. Its production can be shown to be always positive and stops at equilibrium [13].

The stochastic approach allows a more refined description in the GC ensemble. For instance, the atom probability distribution for the momentum mode is determined from the solution of Eq.(19) and corresponds to a Poisson distribution:

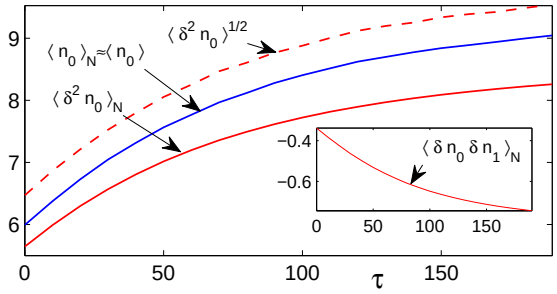

FIG. 2. Evolution of the CN and GC mean atom number in the zero mode and their fluctuations vs. the reduced time τ. The negative correlation with the first excited mode is shown in the inset.

$$P(n_p) = \int \frac{d^2\alpha_p}{\pi} \frac{|\alpha_p|^{2n_p}}{n_p!} e^{-|\alpha_p|^2} P_q = \frac{\overline{n}_p^{n_p}}{(\overline{n}_p+1)^{n_p+1}} \quad (20)$$

with the larger fluctuations $\langle \delta^2 n_0 \rangle_{GC} = \overline{n}_0(\overline{n}_0 + 1)$. Correlations between modes are non existent e.g. $\langle \delta n_0 \delta n_1 \rangle_{GC} = 0$ where n_1 is the mode for the first excited state $k = 2\pi/L$.

The situation changes drastically in a canonical description as the fixed atom number restricts the possibility of fluctuations. Using the formulae (4) and (5) over a sample of 10^6 variables for the stochastic process (1), if the average value remains practically unchanged, the fluctuations are significantly reduced as shown as in Fig.2. The process of evaporative cooling has the effect to increase these fluctuations together with the mean popu-

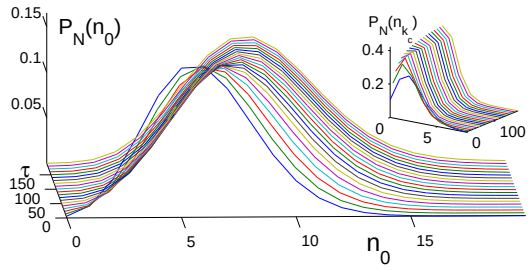

FIG. 3. Evolution of the CN atom probability distribution function in the zero mode vs. the reduced time τ. For comparison, the distribution for the mode k_c is represented in the inset.

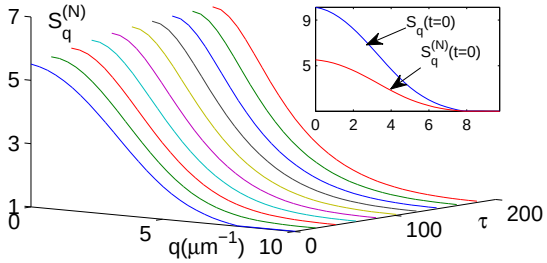

FIG. 4. Evolution of the static structure factor $S_q^{(N)}$ in the CN ensemble. For comparison, the corresponding GC function $S_q(t=0)$ is represented in the inset.

lation. The negative values of $\langle \delta n_0 \delta n_1 \rangle_{CN}$ is an evidence of correlations between modes in the CN ensemble.

The canonical probability distribution resembles a Gaussian one. Fig.3 shows how this distribution evolves with time and illustrates the benefit of using a stochastic approach for quantities that differ according ensembles. For the mode k_c, the distribution is initially peaked and becomes monotonic during the time evolution.

The static structure factor is defined in GC and CN ensembles respectively as [14]:

$$S_q = \langle \delta\rho_q \delta\rho_{-q} \rangle / N \quad S_q^{(N)} = \langle \delta\rho_q \delta\rho_{-q} \rangle_N / N \qquad (21)$$

and corresponds to the density fluctuations $\rho_q = \sum_k c^\dagger_{k-q} c_k$. These functions can be measured in Bragg spectroscopy experiments [15] and reach unity for large momentum q. In Fig.4, we determine the time evolution of these fluctuations during the evaporative cooling process. We notice that the presence of correlation in the CN ensemble reduces significantly the static structure factor.

In conclusion, we have reformulated kinetic theory in terms of a stochastic approach where the stochastic variables describe the various momentum modes of the gas. Through a specific weight average, the CN description becomes accessible and shows drastic differences in comparison with the GC one. The method has been used for a one-dimensional gas but is quite general and can be applied to more general cases of higher dimension, including higher order interaction terms or in presence of longitudinal trap confinement.

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